University of Gdańsk

Subject card

Subject name and code	Numerical methods with algorithms for physical sciences, PG_00129569		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
Education level	Master's studies	Subject group	Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	Arabic ENG
Semester of study	4	ECTS credits	2.0
Learning profile	academic	Assessment form	
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Adam Sieradzan	
	Teachers		

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	0.0	0.0	30
	E-learning hours included: 0.0						

Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
	Number of study hours	30	5.0	15.0	50

Subject objectives	Familiarizing the students with the numerical algorithms applied in chemistry. Preparing the students to write own numerical applications, including existing numerical libraries in the procesess.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student describes floating point arithmetic's problems and explains the causes and implications of floating point round-offs. Defines the concept of the algorithm. Describes the basic numerical algorithms applied in solving equations and systems of linear and nonlinear equations, target function minimization and solving the initial and boundary problems for ordinary and partial differential equations, respectively. The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry	[SW2] presentation/project/paper/ report
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry.	[SW2] presentation/project/paper/ report
[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the responsibility for his/her personal account on the workstation.	[SK1] oral statement/conversation/ discussion [SK2] presentation/project/paper/ report
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the ability of working in a team.	[SK1] oral statement/conversation/ discussion [SK2] presentation/project/paper/ report [SK8] observation of student's independent or team work
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student defines and solves problems related to the specifics of floating point arithmetic that arise when using available packages of quantum chemistry, molecular mechanics and dynamics, chemometrics, etc, The student solves computational problems that arise in chemistry and related subjects when using software libraries available at computer centers, or on the Internet. For this purpose, the student designs simple numerical applications using in-house or library procedures.	[SU1] oral statement/conversation/ discussion [SU2] presentation/project/paper/ report [SU6] demonstration of practical skills
[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry.	[SW2] presentation/project/paper/ report

<table>
<tr><td>Subject contents</td><td>Algorithm and its correctness. Errors in numerical calculations; Wilkinsons lemmas. Condition number of a problem. Overflow (INF), underflow, NaN.
Interpolation: Lagrange and Newton schemes. Numerical differentiation. Numerical integration: the Newton-Coates and Gauss quadratures. Solution
of linear equations systems: the Gauss, Gauss-Jordan, Cholesky, Householder, and QR algorithms. Solution of eigenvalue problem in quantum
chemistry. Solution of nonlinear equations: the Newton, regula falsi, secant, Pegasus, and bisection algorithms. Solution of systems of nonlinear
equations; calculation of equilibrium concentrations in multicomponent systems as an example. Local minimization of functions in single and several
variables in relation to conformational analysis with molecular mechanics. Introduction to global optimization algorithms and their relation to the
problem of finding the most stable structures of molecules and crystals. Least-squares algorithms in fitting models to experimental data: linear and
nonlinear regression (the Newtona-Gauss, Newtona, i Levenberg-Marquardt methods): application in the determination of equilibrium constants.
Statistical assessment of the goodness of fit and of the confidence levels of the determined parameters. Determination of parameters from noisy or
insufficient data: the maximum entropy method. Algorithm for solving ordinary differential equations: application to chemical kinetics and molecular
dynamics. Algorithms for solving partial differentia equations: applications to the electrochemical analysis (e.g., calculation of cyclic voltamperometry
and polarography profiles) and to the calculation of electrostatic solvation energy of macromolecules. Fourier transformation and its application to the
processing of IR and NMR spectra. Cluster analysis algorithms. Factor analysis algorithms and their application to the decomposition of UV spectra,
QSAR, and conformational analysis.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Introduction to Python programming Basis of calculus and linear algebra, ability to use the LINUX operating system.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>task performance reports</td><td>51.0%</td><td>100.0%</td></tr></table></td></tr>
<tr><td>Recommended reading</td><td><table><tr><td>Basic literature</td><td>Siegmund Brandt, Data Analysis - Statistical and Computational Methods for Scientists and Engineers, Springer 2014
Extracurricular readings
Qingkai Kong, Timmy Siauw, Alexandre Bayen, Python Programming and Numerical Methods
A Guide for Engineers and Scientists, Academic Press 2020</td></tr><tr><td>Supplementary literature</td><td>Python Programming for Arduino - Desai Pratik</td></tr><tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr></table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td></td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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